The mystery behind Schrödinger's first communication: a non-historical study on the variational approach and its implications

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> All physicists agree that the problem of physics consists in tracing the phenomena of nature back to the simple laws of mechanics. But there is not the same agreement as to what these simple laws are. To most physicists they are simply Newton's laws of motion. But in reality these latter laws only obtain their inner significance and their physical meaning through the tacit assumption that the forces of which the speak are of a simple nature and possess simple properties. But we have here no certainty as to what is simple and permissible, and what is not: it is just here that we no longer find any general agreement. Hence there arise actual differences of opinion as to whether this or that assumption is in accordance with the usual system of mechanics, or not. (**Heinrich Hertz**)

1 Introduction

Historically, Erwin Schrödinger arrived at his wave mechanics via HJ theory. As shown by Joas and Lehrer in detail [15], what guided Schrödinger throughout was the 'optical-mechanical analogy'—the theoretical relationship between wave and particle motion found in William Rowan Hamilton's work. The analogy provided the final jigsaw piece in his general project

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to extend classical mechanics and more specifically, to provide a non *ad hoc* theoretical explanation for quantised energy levels of the hydrogen atom and Bose-Einstein statistics.[1] As we know, Schrödinger completed the 'optical-mechanical analogy' by providing a wave equation for de Broglie's matter waves. In simple terms, point particle mechanics is seen as the short wavelength limit of 'wave mechanics', analogous to the eikonal approximation in geometrical optics.[2] In Schrödinger's interpretation, his theory is *wave mechanics* proper—an generalsation of classical point particle mechanics to the motion of the mechanical waves. The physical picture for Schrödinger is that the wave nature of matter is fundamental, and the particle picture emerges only as an approximation, arising as part of the wave picture. This constitutes the first line of approach to understand the conceptual relationship between Schrödinger mechanics[3] and HJ theory and is well known within the literature.[4] I shall denote this the *wave* approach.

Another presentation is provided by de Broglie-Bohm theory. Here, I focus on Peter R. Holland's interpretation of the theory as a casual interpretation [14]. As shown by David Bohm [1], Schrödinger equation can be seen as a HJ like equation coupled with a continuity equation, using $\psi = \rho^{1/2} e^{i\mathcal{S}/\hbar}$:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \frac{\nabla S}{m} \right) = 0 \tag{1}$$

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \left(\frac{\partial \mathcal{S}}{\partial q_i} \right)^2 + V(q_i) + Q = 0 \tag{2}$$

with an extra term in the HJ like equation:

$$Q = -\frac{\hbar^2}{2m\rho^{1/2}} \frac{\partial^2 \rho^{1/2}}{\partial q_i^2} \tag{3}$$

called the quantum potential. Hence Schrödinger mechanics can be recast as equations (1) and (2), plus a further equation of motion

$$\mathbf{p} = \frac{\partial \mathcal{S}}{\partial q_i} \tag{4}$$

for the physical system described by (1) and (2).[5] As Holland pointed out, in this approach Schrödinger mechanics can be seen as a natural development

[1] See Joas and Lehrer [15], pp.342-346.

[2] In reality the relationship is much less straight forward. See Holland [14], pp.238-239.

[3] From now on, I call Schrödinger's theory 'Schrödinger mechanics', to make a clear distinction between the mathematical framework, and his interpretation of it.

[4] See for example Yourgrau and Mandalstam [25], pp.116-127 and Butterfield [4].

[5] If one is to be precise, (1) and (2) are only equivalent to Schrödinger equation if an extra quantisation condition is imposed on $\mathcal{S}$. See [23].

of classical HJ theory by permitting 'internal potentials' in the Hamiltonian, namely, higher order derivatives of $\mathcal{S}$ or ρ. In other words, the key difference between 'classical' and 'quantum' lies in the importance of the quantum potential in describing motion. Thus it should be regarded as a new theory of motion.[6]

Further, in this approach a commitment is made on the nature of ψ. The is based on de broglie's idea that both 'wave' and 'particle' are objectively *real*.[7] This means that both are considered as part of what consists the real physical system described by the theory. Thus de Broglie-Bohm theory is also a new theory of matter.[8] The statistical nature of ψ in this physical picture is only secondary. From this perspective, Schrödinger mechanics is essentially a new theory of matter and motion, formulated using the HJ *language*. I shall denote this perspective the *wave-particle* approach.

The above two approaches are well known attempts that provide a *conceptual* interpretation behind the mathematical connections between HJ theory and Schrödinger's theory. There is however a lesser known third approach which arises out of viewing the very same relationship in a different light. It is not quite unknown because it is based on Schrödinger's first communication on wave mechanics.[9] Since this approach is centered upon the variational principle found in Schrödinger's first paper, I shall denote this approach the *variational* approach. This approach has been abandoned by Schrödinger in favour of the more intuitive picture of wave mechanics. As Wessels pointed out, it might be that the variational principle was merely a device to gain acceptance for the then still largely unfamiliar wave equations.[10] Nevertheless, historically it should be made clear that the variational principle was not the center of Schrödinger's thought, but the wave equations.

However, this does not make it less interesting to ask: can the variational approach stand alone, *without* the wave interpretation? The present paper is an attempt to sketch the details of the variational approach, along with some philosophical justifications behind its plausibility. Since this approach is much less well developed than the other two, the considerations here will only be of a preliminary kind. Without referring to terms of a wave theory,

[6]See Holland [14], pp.61-65.

[7]For the history of the development of this idea, see Bacciagaluppi and Valentini [22] and de Broglie [8, 9, 10].

[8][14], p.63.

[9]See Erwin Schrödinger, *Quantisation as a Problem of Proper Value, Part I*, Annalen der Physik (4), Vol. 79, pp. 361-376, 1926.

[10]See Wessels [24], pp.330-333.

I will restrict myself to investigate into the *conceptual* relationship between the two theories. Let me clarify on the meaning of this task.

The model of a physical theory in this paper is the Hertzian one. A physical theory forms a *picture* (or image) of the world with abstract concepts (or symbols of external objects). Concept are components of a picture. A theory is basically a picture with its own set of abstract concepts, not necessarily having any connection to the empirical world *a priori*. There is only one requirement on a theory: a fundamental connection can be established between empirical observations and the picture, such that the consequences of the picture will allow us to anticipate the consequence in reality.[11] And "it is not necessary that they should be in conformity with the things in any other respect whatever". This forms the basic conception of physical theories here, which I shall call *minimalistic realism*.

With this in mind, the central question studied in this paper is the following: how do abstract concepts in HJ theory relate to those in Schrödinger mechanics? I want to focus especially on the relationship between $\mathcal{S}$ and the wavefunction ψ. Is there any sense in which there is a continuity between the two concepts? Each concept in a physical theory functions as part of the picture it presents. Do they retain their significance in one picture as in the other? If not, what is the difference? Thus my aim is to present the variational approach mentioned above as a fresh attempt to address this central question.

The paper consists of three main sections. First, I will study an interpretation of classical HJ theory that underlies the variational approach. An attempt is made to describe the physical picture presented and presupposed by HJ equation, with a special focus on the meaning of the $\mathcal{S}$ function. Then I will study the possibility of equipping HJ theory with a classical statistical framework and the physical picture it presents. Second, some motivations are given for extending this physical picture and formalism to Schrödinger mechanics. This is emphatically *not* a 'derivation' of Schrödinger's theory. In fact, the emphasis here is that Schrödinger mechanics is conceptually distinct from any form of classical theories. Finally, light will then be shed on the central question set out above.

The contributions of this work are twofold. First, I argue the importance of seeing the concept 'motion' as an abstract concept in Schrödinger mechanics, due to its changed empirical status in subatomic 'quantum' phenomena. However, the more important contribution here lies in the observation that

[11] Thus for example, in Hertz's book the single connection he requires, is through the fundamental law of motion.

the role the 'quantum state' plays in Schrödinger mechanics is conceptually analogous to the role of motion, not the physical state, in classical mechanics. This is the most important insight arising out of the variational approach.

2 Hammilton-Jacobi theory

2.1 Formalism

In general, HJ theory denotes a mathematical theory in the calculus of variation [19]. However, in this section I shall denote by HJ theory the specific application of this method in classical mechanics, especially in solving the problem of dynamics. The method to achieve this is normally known as Jacobi's method. It consists of two steps: first finding a single function $\mathcal{S}(q_i, t; a_i, A)$ that depends on $n+1$ arbitrary algebraically independent constants $(a_1, ...a_n, A)$ by solving the HJ equation

$$\frac{\partial \mathcal{S}}{\partial t} + \mathcal{H} = 0 \tag{5}$$

for a system with a Hamiltonian

$$\mathcal{H} = \mathcal{T} + V = \frac{1}{2m}\left(\frac{\partial \mathcal{S}}{\partial q_i}\right)^2 + V(q_i) \tag{6}$$

where $i = 1, ...n$, n is the number of degrees of freedom. Because $\mathcal{S}$ does not appear explicitly in the HJ equation, one of the constants will be an additive constant. Thus we have:

$$\mathcal{S} = \mathcal{S}(q_i, t; a_i) + A \tag{7}$$

Second, to solve for the motion, i.e finding $q_i = q_i(t)$, we can use Jacobi's law of motion:

$$\frac{\partial \mathcal{S}}{\partial a_i} = b_i \tag{8}$$

Now solve for: $q_i = q_i(t; a_j, b_k)$, for $i, j, k = 1, ...3n$ by algebraic rearrangement. The setting of these constants, for the moment, are entirely arbitrary. However, by identifying the a_i's and b_i's with key physical quantities in the problem, for example the initial positions and momenta of the system, we can recover the form of the well known solutions in classical mechanics. For example, consider a free particle in 1 dimension. It can be shown that

$$\mathcal{S} = \frac{1}{2}m\frac{(q-q_0)^2}{t-t_0} \tag{9}$$

satisfies the HJ equation. If we take q_0 as a_1, then Jacobi's law of motion

$$\frac{\partial \mathcal{S}}{\partial a_1} = \frac{\partial \mathcal{S}}{\partial q_0} = -m\frac{q - q_0}{t - t_0} = b_1 \tag{10}$$

should give us $q = q(t)$ after rearrangement. If we write $b_1 = p_0$, i.e. the initial momentum, we have:

$$q(t) = q_0 - \frac{p_0}{m}(t - t_0) \tag{11}$$

which gives the motion of a free particle in terms of the initial momentum.

However, if we take t_0 as a_1, then

$$\frac{\partial \mathcal{S}}{\partial a_1} = \frac{\partial \mathcal{S}}{\partial t_0} = \frac{1}{2}m\frac{(q - q_0)^2}{(t - t_0)^2} = b_1 \tag{12}$$

which again, gives $q_i = q_i(t)$. If we write $b_1 = E$, i.e. the energy, we have:

$$q(t) = q_0 + \sqrt{\frac{2E}{m}}(t - t_0) \tag{13}$$

which given the motion of a free particle in terms of the energy.

HJ equation is a partial differential equation which means there are infinitely many solutions. The importance of Jacobi's method is that it provides a way to find the set of $\mathcal{S}$ that are actually relevant to the problem of motion. Using the above procedure, actual motion can be constructed using the solutions of the HJ equation. This way, HJ equation can be seen as a theory of motion in classical mechanics. I will now turn to discuss the conceptual significance of HJ theory now.

2.2 Conceptual Interpretation

2.2.1 Levels of the dynamical problem

In what sense does HJ theory solve the problem of motion? Here, it is important to point out that HJ theory is radically different from the perspective of Newtonian or variational mechanics in dealing with dynamics. In these approaches, the theory describes dynamics of a physical system by providing its trajectory via an equation of motion. The initial data is specified in order to determine the unique motion of the system. HJ theory, however, provides a much more general solution to the problem of dynamics. This is because in solving for $\mathcal{S}$, dynamics is provided at a level before any equation of motion is even derived. It is true that the equation of motion is contained when we have solved for $\mathcal{S}$ via Jacobi's law of motion. However, this distinction is important when we get to Schrödinger mechanics because there, the challenge is to find a physical theory that describes the observations in subatomic physics with a dynamical framework, *without* committing to a particular equation of motion or exact dynamics. Thus we can already see HJ theory is particular well suited for constructing a theory of subatomic physic. So for the moment, let us distinguish different conceptual levels of a dynamical problem by the following schema:[12]

Level	Significance
1	Determination of general dynamics
2a	Determination of equation of motion
2b	Specification of initial data
3	Determination of exact motion (trajectory)

Within this schema, the determination of $\mathcal{S}$ via the HJ equation is at level 1. Arriving at an equation of motion is at level 2a. $\mathcal{S}$ together with the specification of the integration constants is at level 2b. At level 3, the whole path of motion $q_i = q_i(t)$ is determined.

With the above schema, we can understand better the conceptual relationship between HJ theory and other formulations of classical mechanics. The critical difference lies in the extend of 'determination' at level 1. In HJ theory, the general dynamics for a physical system with a given Hamiltonian $\mathcal{H}$ is completely determined. It is general, in the sense of without the restriction to consider a particular equation of motion/trajectory. In other formulations of mechanics an equation of motion is the central equation and thus the description is restricted to a particular trajectory, and therefore at level 2a.[13]

Further, this schema shows us that there are different 'levels' of determination in dynamics. The important consequence is that the physical picture presupposed at each level is different. In HJ theory, for example, we have a framework for specifying dynamics in a general sense, without committing to follow a particular single trajectory. Thus at level 1a, the picture there is not of an individual physical system with a trajectory and an initial state. These only come at subsequent levels. By separating the determination of

[12] My approach here is different, but I hope, complementary, to the insightful discussion in Butterfield [5].

[13] Albeit particular not in the sense of *exact*, because no restriction is placed on the choice of initial data. Particular means that it follows *one* potential trajectory, rather than many potential trajectories. The latter is true of the action principle, for example, where many virtual trajectories are considered.

dynamics into a few levels, we can see more clearly the appropriate physical picture presupposed by each level.

2.2.2 The physical meaning of $\mathcal{S}$ and the Hamilton-Jacobi equation

The central question then is the following: what is the conceptual significance of the HJ equation? In other words, what is the physical problem posed, and the physical picture presupposed by the equation? The HJ equation is an equation for the function $\mathcal{S}$, which is a function on configuration space and so there is not an obvious physical interpretation of $\mathcal{S}$.[14] There are three different approaches to answer this question. The first approach is the historical one, namely, that HJ theory presents a picture to unify wave and particle motion. The second approach is a common one found in textbooks, namely, that HJ theory is concerned with generating functions for canonical transformations. The third approach is a less common one, which can be found in Butterfield [5], Cook [6, 7], Holland [14] and Landauer [17]: HJ theory refers to an ensemble of fictitious particles on fictitious trajectories.

In the first picture, the physical problem posed for the HJ equation is to find the 'guiding' wave fronts for particle motion. This can only be understood if we set this approach within the context of Hamilton's work. Hamilton was initially concerned with geometrical optics. For Hamilton, his task was to find a single mathematical function such that all the paths for light in a given environment can be derived from this single function. Let us denote this function Hamilton's characteristic function $\mathcal{S}_{\mathcal{H}}$. The physical significance of this function was to describe the family of surfaces in Malus' theorem—"that for any bundle of light rays emitted from a point, there will be a family of surfaces so that all light rays are orthogonal to these surfaces."[15] Thus the HJ equation solves for a function which characterises a family of surfaces. Jacobi's law of motion can then be used to find the particle/ray trajectory from this one single function, given the necessary initial data. This is the picture that led to Schrödinger's wave interpretation of his theory.

In the second picture, the physical problem posed for the HJ equation is

[14] It is often noted that $\mathcal{S}$ is the action in mechanics textbooks. This is true only to the extend that the action is one of the solution that works in the HJ method. However, HJ method is not restricted to using the action as the only possible means to solve the problem of motion.

[15] See Joas and Lehrer [15], p.340. For more details, see Butterfield [4].

to find out the generating functions for canonical transformations.[16] Recall the physical significance of canonical transformations is that they produce the true motions connecting two physical states. The generating function for canonical transformations thus can be seen as generator of mechanical paths connecting an initial state (q_i, p_i) to a final state (Q_i, P_i). The problem of motion in HJ theory can then be phrased as the following: given a system with a Hamiltonian $\mathcal{H}$, what is the generating function $\mathcal{S}$ that gives rise of canonical transformations? The answer is that $\mathcal{S}$ must satisfy the HJ equation. This picture is connected with Dirac's well known work on transformation theory in quantum mechanics by treating the commutators as the quantum mechanical equivalent of the Poisson brackets.

However, a third picture is possible. In this picture, the problem posed for the HJ equation is to find the dynamics of a physical system at level 1 in the above schema. It refers to an ensemble of fictitious particles on potential actual trajectories. I shall call this an *Hamilton-Jacobi ensemble*, to distinguish it from any other concepts of ensemble in SM. Conceptually, this means that HJ theory treats the whole configuration space as points on potential actual trajectories. Solving the HJ equation for $\mathcal{S}$ gives rise to all the actual dynamical possibilities associated with each point in configuration space for a given $\mathcal{H}$. How does this work?

First, notice that the HJ equation solves for a field $\mathcal{S}$ such that it provides the dynamics for each point q_i in configuration space, *if it happens to be found in the state* q_i. $\mathcal{S}$ provides a field on configuration space where the dynamics can be derived readily through $\frac{\partial \mathcal{S}}{\partial q_i}$ at each point.

However, the general solution for the equation does not commit to describe any particular particle trajectories with a particular set of initial data. This occurs only at level 2. Further, HJ equation contains as many constants of integration as there are degrees of freedom, and these can be chosen arbitrarily, as shown previously. The specification of these constants occur also only at level 2. Thus solving the HJ equation provides dynamics in the most general sense (level 1): *if* a particle happens to be found in the state q_i, its dynamics at that point is $\frac{\partial \mathcal{S}}{\partial q_i}$.

This is rather significant because as seen in the above way, HJ theory should be regarded as a *framework* for dynamics. HJ theory is a dynamical framework serving as a background for further determination of the solution to the problem of motion. For example, the solution for the free particle trajectory found in the previous section can be seen conceptually as consist of two steps. First, as an application of HJ theory as a general dynamical

[16] See Lanzcos [16],pp.216-239 and Holland [14], pp.29-33.

framework by finding a $\mathcal{S}$ that satisfies the HJ equation. Second, by specifying the integration constants as initial momentum/Energy, we arrive at the exact for of the actual motion. Conceptually speaking, only when the second step is taken have we turned from an ensemble of fictitious particles on potential actual trajectories, to a specific actual particle on a definite trajectory.

2.3 HJ theory with a statistical framework

With the third picture in mind, there is an obvious possibility of equipping HJ theory with a statistical framework. If HJ equation refers to an ensemble of fictitious particles on possible actual trajectories, then just as in statistical mechanics (SM), we can equip the ensemble with a probability distribution.[17]

However, we must be really careful here. What is the physical significance of the HJ ensemble? It is very similar to the notion of a Gibbsian ensemble. This means that the members of the ensemble are strictly fictitious, i.e. they have no real empirical reality attached to them. The connection to empirical reality is done through the statistical averages over the ensemble, as in the case of Gibbsian SM.

2.3.1 Conceptual Foundation

In classical mechanics, a specification of the system's state is given by (q_i, p_i). Given the state, as well as the Hamiltonian of the system $\mathcal{H}$, one can solve the HJ equation and obtain $\mathcal{S}$, which completely solves the possible motion of the system. Now classical SM applies to situations where a specification of the exact state of the system is not possible. It allows one to take into account the lack of knowledge we have about the system and consequently make statistical predictions during experiments. In classical SM, one usually uses the notion of a phase space, which is a $2n$ dimensional space where each point (q_i, p_i) corresponds to a possible state one can find the representative point. Here, n is the degrees of freedom in the physical system under consideration. This is convenient because in phase space one can assume each point evolves according to Hamilton's equations, and so given an ensemble of states, i.e. a region of phase space, we can assume each member of the ensemble evolves according to the same dynamics. As a consequence, the probability distribution over phase space, $F(q_i, p_i, t)$ which assigns probability of finding a representative point to be in a particular state, evolves

[17] I follow Tolman [21] here on the conception and presentation of classical SM.

according to Liouville equation:

$$\frac{dF(q_i, p_i, t)}{dt} = 0 \tag{14}$$

which follows from Hamiltonian mechanics. The important observation to make is that any allowed distribution must satisfy Liouville equation, which is an implication of Hamiltonian dynamics. In classical SM, the dynamics of the state is entirely *independent* of the specification of initial distribution. In other words, different distributions will consist of states that evolve according to the same dynamics. As we will see, this marks the critical difference between classical SM and Schrödinger mechanics.

2.3.2 Formalism

Now we can consider equipping a classical statistical framework in configuration space for the HJ picture sketched in the previous section. Recall $\mathcal{S}$ refers to an ensemble of fictitious particles. We can equip a statistical framework on this picture via the following question: what is the probability of q_i being the configuration of the representative point? In other words, what is the probability of q_i being found on the motion of the representative system?

Notice that the above question is formulated at level 1. This means that no assumption is yet made about the actual trajectory of the representative point. The only question is that the representative point *has actual motion in principle*. From the context of the question formulated, it is intuitive that the actual motion in principle should have an effect on the probability distribution. This can be seen later in the presence of $\frac{\partial \mathcal{S}}{\partial q_i}$ in the continuity equation.

With the above question in mind, we can formulate a classical statistical framework in the following way. A state in configuration space is specified by q_i. The number of states N in the ensemble is given by:

$$N = \int ... \int \rho(q_i; t) dq_1 ... dq_n \tag{15}$$

where n is the degree of freedom and $\rho(q_i; t)$ is the probability distribution on the ensemble. Now

$$\frac{\rho(q_i; t)}{N} = \frac{\rho(q_i; t)}{\int ... \int \rho(q_i; t) dq_1 ... dq_n} \tag{16}$$

is the probability per unit volume in configuration space for the representative point to be found at q_i at time t. If we apply the normalisation condition:

$$\int ... \int \rho(q_i;t)dq_1...dq_n = 1 \tag{17}$$

then $\rho = \rho(q_i;t)$ gives directly the probability per unit volume in configuration of finding the representative point at q_i at time t. This is convenient and from now on we will assume this is always imposed. Now any mechanical quantity $F(q_i;t)$ has a *mean value* over the ensemble of states given by:

$$\langle F \rangle = \int ... \int F(q_i;t)dq_1...dq_n \tag{18}$$

This defines the average value for any mechanical quantities over the ensemble. It is averaged over all the possible states. The evolution of the probability distribution is given by the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \frac{\nabla \mathcal{S}}{m} \right) = 0 \tag{19}$$

which can be shown through some elementary considerations.[18] Thus for a given classical mechanical system with dynamics characterised by $\mathcal{S}$, the distribution ρ used to equip a statistical framework for a HJ ensemble must satisfy the continuity equation. We shall call the above framework *statistical HJ theory.*

As shown by Cook [7] and Holland [14], statistical HJ theory can be beautifully summarised by a variational principle

$$\delta \int dq_1...dq_n \left\{ \rho \left[\left(\frac{\partial \mathcal{S}}{\partial t} + \mathcal{H} \left(q_i, \frac{\partial \mathcal{S}}{\partial q_i} \right) \right) \right] \right\} = 0 \tag{20}$$

by treating $-\rho$ and $\mathcal{S}$ as conjugate variables. The HJ equation and the continuity equation are then derived as the Euler-Lagrange equation for the variational principle. As we will see, it is precisely this variational principle which provides a physical motivation behind the variational approach in Schrödinger's first communication.[19]

[18] See [14], pp.46-47

[19] This connection is observed by Joas and Lehrer [15], p.346: "In the text corresponding to this item, Schrödinger starts from the Hamiltonian partial differential equation and reinterprets it as a variational principle which indeed leads him to the (nonrelativistic) wave equation."

3 Extending the picture

3.1 An arbitrary change of variable or a generalised framework for statistical HJ theory?

We will now provide some motivations to see Schrödinger mechanics as a statistical HJ theory. In the spirit of HJ theory, the main physical content in statistical HJ theory should be specified by 1 single function only. Denoting this function by ψ, consider the following change of variable:

$$\mathcal{S} = K ln\psi \qquad \psi = exp(\mathcal{S}/K), \qquad \psi \in \mathbb{R} \tag{21}$$

where K is a constant with the dimension of action. This is necessary since ψ must be dimensionless inside the logarithm. Notice that this is the famous *ad hoc* looking transformation introduced by Schrödinger in his first paper on wave mechanics. With this change of variable, we have the following identities:

$$\frac{\partial \mathcal{S}}{\partial q_i} = \frac{K}{\psi}\frac{\partial \psi}{\partial q_i}, \qquad \frac{\partial \mathcal{S}}{\partial t} = \frac{K}{\psi}\frac{\partial \psi}{\partial t} \tag{22}$$

$$\frac{\partial \psi}{\partial q_i} = \frac{\psi}{K}\frac{\partial \mathcal{S}}{\partial q_i}, \qquad \frac{\partial \psi}{\partial t} = \frac{\psi}{K}\frac{\partial \mathcal{S}}{\partial t} \tag{23}$$

Substituting back into the HJ equation, we have:

$$\mathcal{H}\left(q_i, \frac{K}{\psi}\frac{\partial \psi}{\partial q_i}\right) = E \tag{24}$$

which becomes:

$$\frac{K^2}{2m}\left(\frac{\partial \psi}{\partial q_i}\right) + V(q_i)\psi^2 = E\psi^2 \tag{25}$$

Now if we transform the only the derivatives back to $\mathcal{S}$, the equation has a very suggestive form:

$$\frac{1}{2m}\left(\frac{\partial \mathcal{S}}{\partial q_i}\right)^2 (\psi^2) + V(q_i)(\psi^2) - E(\psi^2) = 0 \tag{26}$$

The left hand side looks like the integrand of the variational principle above, if we identify $\rho = \psi^2$.[20] Recall that the content of statistical HJ theory can be summarised by the variational principle. Thus the famous 'arbitrary' looking transformation can be motivated by the following requirement: *to*

[20] Recall in HJ theory, $E = -\frac{\partial \mathcal{S}}{\partial t}$, and $\mathcal{H} = \frac{1}{2m}\left(\frac{\partial \mathcal{S}}{\partial q_i}\right)^2 + V(q_i)$.

look for a single function to describe all the physical content in statistical HJ theory.[21] This is the starting point of the variational approach.

So far, the transformation is obviously inadequate for this requirement since we have two real functions $\mathcal{S}$ and ρ but only 1 real function ψ. In order to express all the physical information in statistical HJ theory by one single function, ψ must be complex. Combining with the above heuristic motivation, we have the following *definition*:

$$\psi = \rho^{1/2} exp(\mathcal{S}/K), \qquad \qquad \psi \in \mathbb{C} \tag{27}$$

which amounts to the polar representation of a complex variable if and only if $K = \pm i\hbar, \hbar \in \mathbb{R}$.[22] We choose $K = -i\hbar$ from now on.

With this definition, it seems now we have a single function that carries both the dynamics and the probability distribution. Let us investigate what this change entails. For convenience, let $R = \rho^{1/2}$. Consider

$$ln\psi = ln(Rexp(i\mathcal{S}/\hbar)) \tag{28}$$

which becomes:

$$ln\psi = lnR + i\mathcal{S}/\hbar \tag{29}$$

So the expression for $\mathcal{S}$ is given by:

$$\mathcal{S} = i\hbar lnR - i\hbar ln\psi \tag{30}$$

Recall the expression for momentum in HJ theory is $\frac{\partial \mathcal{S}}{\partial q_i}$. Using the expression for $\mathcal{S}$ above, we get:

$$\frac{\partial \mathcal{S}}{\partial q_i} = \frac{i\hbar}{R}\frac{\partial R}{\partial q_i} - \frac{i\hbar}{\psi}\frac{\partial \psi}{\partial q_i} = \frac{i\hbar}{2}\frac{\partial lnR^2}{\partial q_i} - \frac{i\hbar}{\psi}\frac{\partial \psi}{\partial q_i} \tag{31}$$

We can see that unlike in the previous case where ψ is real, by making ψ complex the transformation is not just a change of variable. It modified the expression for the momentum by introducing a new R derivative term. This means that part of the theory that describes the dynamics has significantly changed, where it could be dependent on the specification of the probability distribution. Further, it is not even straight forward to think of $\frac{\partial \mathcal{S}}{\partial q_i}$ as an

[21] What is demonstrated in this section is by no means equivalent to explaining the exact physical meaning of the transformation. However, it does provide some motivations behind the variational approach.

[22] $\hbar$ here is merely a 'suggestive' constant. The empirical content of the theory is entirely justified by experimental verification, including the value of $\hbar$.

expression for momentum now, since the first term is certainly complex and so $\frac{\partial\mathcal{S}}{\partial q_i}$ is in general a complex expression.[23]

Further, if we consider:

$$\mathcal{S} - i\hbar ln R = \mathcal{S}' = -i\hbar ln\psi, \qquad\qquad \mathcal{S}' \in \mathbb{C} \tag{32}$$

then the transformation can be seen as a change of complex variable $\mathcal{S}'$ to ψ. By considering the introduction of ψ into statistical HJ framework in the perspective of $\mathcal{S}'$ we obtain an important insight. This new framework can be cast as a HJ framework, albeit with the complex $\mathcal{S}'$ as defined above, instead of the real $\mathcal{S}$ in classical HJ theory. Thus if we replace all the $\mathcal{S}$ by $\mathcal{S}'$ we obtain a new framework, characterised by the use of a complex variable in the old familiar language of the last section. The key, however, is to notice that the meaning of expressions in this new framework such as $\frac{\partial\mathcal{S}'}{\partial q_i}$ *is certainly not equivalent to* $\frac{\partial\mathcal{S}}{\partial q_i}$*, which can be interpreted simply as momentum. This is due to the fact that the familiar looking expression* $\frac{\partial\mathcal{S}'}{\partial q_i}$ *is now in general complex.*

3.2 Schrödinger mechanics

3.2.1 From classical statistical mechanics to Schrödinger mechanics

I will now discuss the physical significance of Schrödinger mechanics in the variational approach. Recall that in classical HJ theory, dynamics of individual states is equivalent for different statistical ensembles chosen. This is justified by the fact that dynamics is an empirical law since the motion of planets and macroscopic objects are considered as observed directly. Thus the law of motion is taken as the only 'empirical law' of nature in classical mechanics, as Hertz observed [13]. Rightfully, 'classical' statistical ensemble considers a collection of systems where their dynamics is taken as governed by the empirical laws of classical mechanics. This is seen by the fact that HJ equation is independent of ρ, and so the dynamics is solely determined by $\mathcal{S}$.

However, at subatomic level trajectories are not observed directly in experiment and thus should be regarded as an abstract concept in the theory,

[23] Unless the extra term vanish, which amounts to some 'recovery' of the classical version of statistical HJ theory. There are two ways to recover a classical statistical theory from this framework: i) $\hbar \to 0$, ii) $\frac{\partial ln R^2}{\partial q_i} = 0$. But as Holland pointed out ([14], p.219), $\hbar \to 0$ is a difficult statement to interpret, since against what scale or in what precise physical circumstances should we regard $\hbar$ as small?

in the Hertzian sense. Only localisation of particles (e.g. electrons, photons) are observed directly, as pointed out by de Broglie [10]. Further, what is obtained from the early quantum experiments are the position/energy distributions and discrete energy 'levels'. The correct distribution of localisation is what is required of the theory to describe at subatomic level, not the trajectories. This motivates the central key assumption behind Schrödinger mechanics, namely that states in an ensemble need not be governed by an universal dynamics.

Schrödinger mechanics can be seen as an implementation of this change of view. A convenient schema is provided by the above generalised statistical HJ theory. A dramatic consequence follows, namely that the determination of dynamics is not the central empirical problem in the theory. Instead, determination of ψ becomes the non-trivial empirical problem in the theory, since it is now impossible to determine the dynamics for states in the ensemble first, and then assign a distribution on the ensemble. The major change in Schrödinger mechanics amounts to this lost of independence for dynamics as a concept, and hence the non-trivial usefulness of using 1 single function in statistical HJ theory. With this in mind, we are now ready to elucidate the physical meaning of standard features in the theory.

3.2.2 Schrödinger Densities—'Operators'

The relevant physical quantities in Schrödinger mechanics are introduced as follows. As in any statistical theory, in general the quantities with empirical significance are not the local values, but averages over an ensemble of dynamical states. Nevertheless, the local values are abstract concepts used to formulate averages. So we must first define densities for dynamical variables.

The density for a physical quantity is defined by the local value multiplied by the distribution of states in a HJ ensemble. Thus the densities $d_{\mathcal{A}}$ is defined as:

$$d_{\mathcal{A}} = \mathcal{A}\rho = \mathcal{A}|\psi|^2 \tag{33}$$

For example, the local energy density is given by:

$$d_E = |\psi(q_i, Q_i, t)|^2 \left(-\frac{\partial \mathcal{S}'}{\partial t}\right) = \psi^* \left(i\hbar\frac{\partial}{\partial t}\right)\psi \tag{34}$$

and finally the local momentum density:

$$d_{p_i} = |\psi(q_i, Q_i, t)|^2 \left(\frac{\partial \mathcal{S}'}{\partial q_i}\right) = \psi^* \left(-i\hbar\frac{\partial}{\partial q_i}\right)\psi \tag{35}$$

Now we can use these basic quantities to form more complicated quantities. For example, the local kinetic energy density is given by:

$$d_{\mathcal{T}} = |\psi(q_i, Q_i, t)|^2 \frac{1}{2m} \sum_{i=1}^{n} \left(\frac{\partial \mathcal{S}'}{\partial q_i} \right)^2 = \frac{\hbar^2}{2m} \sum_{i=1}^{n} \left| \frac{\partial \psi}{\partial q_i} \right|^2 \tag{36}$$

and the local Hamiltonian density are given by:

$$d_{\mathcal{H}} = |\psi(q_i, Q_i, t)|^2 \mathcal{H} \left(q_i, \frac{\partial \mathcal{S}'}{\partial q_i} \right) = \frac{\hbar^2}{2m} \sum_{i=1}^{n} \left| \frac{\partial \psi}{\partial q_i} \right|^2 + V(q_i)|\psi|^2 \tag{37}$$

We interpret these densities as densities over the HJ ensemble. They are *not* physical densities, unlike for example particle densities in a gas. They are fictitious densities used to compute *physical* quantities, namely the statistical averages. But they are *not* probability densities.[24]

As we can see, the form of the energy and momentum densities resembles the mysterious 'operators'![25] From this perspective, we can see a clear physical meaning behind the operators, in relation to the language of statistical HJ theory.[26]

3.2.3 Averages over a HJ ensembles—'Expectation values'

With the local densities, we can now define averages or mean values for physical quantities. *The average of a physical quantity over a HJ ensemble is defined by integrating the local densities over all the possible states.* Thus we have:

$$\langle \mathcal{A} \rangle = \int d_{\mathcal{A}} dq_1 ... dq_i \tag{38}$$

For example, the average momentum is given by:

$$\langle p_i \rangle = \int d_{p_i} dq_1 ... dq_i = \int \psi^* \left(-i\hbar \frac{\partial}{\partial q_i} \right) \psi dq_1 ... dq_i = \int \psi^* \hat{P}_i \psi dq_1 ... dq_i = \langle \hat{P}_i \rangle \tag{39}$$

which is the expectation value of the momentum operator! We can see that the expectation value of operators are found to have empirical significance

[24] As Cook noted, these densities are not in general probability distributions, since they can be negative and do not necessarily obey the Kolmogorov axioms. See [7], pp.135-136.

[25] The introduction of the Hamiltonian operator is less obvious. As we can see, the Hamiltonian operators do not enter the theory via having the exact form as the Hamiltonian density. I will not go into the details here but see [7], pp.154-158 for an extended discussions.

[26] For a detailed discussion, see [6], p.81-88.

in the standard formalism, precisely because they are the physical averages in a statistical HJ framework. In a statistical theory, these are the obvious quantities with empirical significance.

3.2.4 Schrödinger's Variational Principle—Schrödinger equation

We now require a law to select all the possible ψ allowed in the theory. This law can be treated as the sole physical hypothesis in Schrödinger mechanics, which requires empirical verification. We have already seen that classical statistical HJ theory can be derived from a variational principle. The physical meaning of the variational principle is further clarified by noting that it is equivalent to:

$$\int dq_1...dq_i d_E = \int dq_1...dq_i d_{\mathcal{H}} \tag{40}$$

where in the classical theory, $\rho = R^2, d_E = -\rho\frac{\partial\mathcal{S}}{\partial t}, d_{\mathcal{H}} = \rho\left(\frac{(\nabla\mathcal{S})^2}{2m} + V\right)$. Thus the physical content of the statistical HJ theory is equivalent (up to boundary conditions) to asserting the following:

> *The average energy is equivalent to the average Hamiltonian over the HJ ensemble.*

I shall call this *Schrödinger's variational principle*, since this is exactly the same principle he proposed in the first communication to replace the quantisation conditions.

In Schrödinger mechanics, we still have the same principle but instead of $\mathcal{S}$, we have $\mathcal{S}'$ instead:

$$\delta\int dq_1...dq_i\left\{\left[\rho\left(\frac{\partial\mathcal{S}'}{\partial t} + \mathcal{H}(q_i, \nabla\mathcal{S}')\right)\right]\right\} = 0 \tag{41}$$

Now using the transformation between $\mathcal{S}'$ and ψ, we can rewrite the variational principle in terms of ψ and ψ^*. Vary with respect to ψ^* (or ψ), we obtain the Schrödinger equation for ψ (or ψ^*):[27]

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2\psi + V\psi \tag{42}$$

Schrödinger's variational principle is the only constraint on ψ.[28] Now the physical problem in this generalised dynamical framework becomes solving

[27] For the full derivation, see [6], p.63-68.

[28] Notice that this is not strictly true, if one considers the single-valuedness of ψ, the behaviour on the boundaries...etc as extra constraints.

for ψ, instead of ρ and $\mathcal{S}$ separately. Thus solving for ψ seems to amount to solving for possible HJ ensembles that will occur in nature. Moreover, in general, these ensembles have states evolving according to non-classical motions.

4 Elucidations

4.1 HJ theory as a common language

4.1.1 What is the 'momentum'?

We are now in a position to discuss how the variational approach answers the central question raised at the beginning of the paper, namely, what is the conceptual relationship between the abstract concepts in HJ theory and Schrödinger mechanics. We can see that HJ theory is a framework for dynamics both in classical mechanics and Schrödinger mechanics. The major continuity between classical and Schrödinger mechanics lies within the presence of a common language.

However, this continuity is actually more confusing than it seems. Consider the expression for momentum averages over a HJ ensemble:

$$\langle p_i \rangle = \int d_{p_i} dq_1 ... dq_i = \int \psi^* \left(-i\hbar \frac{\partial}{\partial q_i} \right) \psi dq_1 ... dq_i = \int \psi^* \hat{P}_i \psi dq_1 ... dq_i = \langle \hat{P}_i \rangle \tag{43}$$

This is one of the many clarifications from this perspective. We have a well motivated explanation as to why operators can be introduced into QM. They are the densities for a dynamical variable in a HJ ensemble. Notice though that this explanation works, only if the substitution for ψ is possible in d_{p_i}. However, the substitution for ψ comes from:

$$\frac{\partial \mathcal{S}'}{\partial q_i} \tag{44}$$

not

$$\frac{\partial \mathcal{S}}{\partial q_i} = \frac{-i\hbar}{\psi} \frac{\partial \psi}{\partial q_i} + \frac{i\hbar}{R} \frac{\partial R}{\partial q_i} \tag{45}$$

As we can see, in general there is a second term dependent on R in $\frac{\partial \mathcal{S}}{\partial q_i}$. So the quantity d_{p_i} should not really be interpreted as a 'momentum' density, and $\int d_{p_i} dq_1 ... dq_i$ be interpreted as 'average momentum', unless we are willing to call the derivative of the complex variable $\mathcal{S}'$ a 'momentum'.

The issue here is whether there is a meaningful candidate for momentum in Schrödigner mechanics. De Broglie-Bohm theory indeed realised that $\frac{\partial \mathcal{S}}{\partial q_i}$

is such a candidate. However, from our detailed study of the HJ framework, in general this is not actually the natural 'momentum'. If we follow through the construction of Schrödinger mechanics, the natural expression is $\frac{\partial \mathcal{S}'}{\partial q_i}$. How does de Broglie-Bohm theory work?

The reason it works is the following. Consider the local momentum density in classical HJ theory:

$$d_{p_i} = R^2 \frac{\partial \mathcal{S}}{\partial q_i} \tag{46}$$

This quantity, in the generalised framework, becomes:

$$R^2 \frac{\partial \mathcal{S}}{\partial q_i} = \psi^* \left(-i\hbar \frac{\partial}{\partial q_i} \right) \psi + \frac{i\hbar}{2} \frac{\partial R^2}{\partial q_i} \tag{47}$$

If we consider the average 'momentum' by integrating, we have

$$\langle p_i \rangle = \int R^2 \frac{\partial \mathcal{S}}{\partial q_i} dq_1 ... dq_i = \int dq_1 ... dq_n \int \left[\psi^* \left(-i\hbar \frac{\partial}{\partial q_i} \right) \psi + \frac{i\hbar}{2} \frac{\partial R^2}{\partial q_i} \right] dq_i \tag{48}$$

Now the second term vanishes, if we impose that $R^2 = \rho$ vanishes at the boundary:

$$\int dq_1 ... dq_n \int \frac{i\hbar}{2} \frac{\partial R^2}{\partial q_i} dq_i = const \times \left[R^2 \right] \to 0 \tag{49}$$

Hence,

$$\langle p_i \rangle = \int R^2 \frac{\partial \mathcal{S}}{\partial q_i} dq_1 ... dq_i = \int dq_1 ... dq_n \int \psi^* \left(-i\hbar \frac{\partial}{\partial q_i} \right) \psi = \langle \hat{P}_i \rangle \tag{50}$$

Thus, the so called de broglie-Bohm 'momentum' is the correct momentum, only when considered at the level of the averages.[29]

We can see that although a HJ framework is used in Schrödinger mechanics, its physical meaning at the ground level has changed significantly. At the level of local values, it is not possible to say that there is a physically meaningful 'momentum' in the generalised framework, sketched in section 3. The 'momentum' averages are physically meaningful, and they are constructed by using the 'right' kind of expressions, such as $\frac{\partial \mathcal{S}'}{\partial q_i}$. But since in general these quantities are complex, it is difficult to interpret the actual physical meanings of their values.

[29] I believe this is connected to Basil Hiley's observation that Bohm's momentum is identical to the 'weak value', which is an averaged quantity not a local value (Through private communication).

4.1.2 Analogy between 'motion' and 'quantum state'

It seems that there are two options regarding the meaning of the HJ framework in Schrödinger mechanics. First, the HJ framework functions in a similar way as in classical mechanics, although at the level of the averages. The explanation for quantum phenomena is given through a commitment to provide an underlying physical picture at the level of motion for physical phenomena. This amounts to de Broglie-Bohm theory's perspective. Second, the HJ framework functions as a way to write down a theory whereby the empirical data obtained from quantum phenomena can be explained in a way, *without committing to an underlying physical picture at the level of motion.*

The main fruit arises from the variational approach is that an interpretation taking the second option can be constructed with conceptual clarity. The main idea can be summarised as follows: *The dynamics of a physical system, if relegated from the status of an empirical law, is not a necessary part of a physical picture. Instead, the empirical law in Schrödinger mechanics concerns the 'quantum state', ψ. Thus the 'quantum state' as a concept has an analogous role to motion in classical mechanics, in the physical picture behind an explanation of quantum phenomena. It is in this sense that the 'quantum state' is said to correspond to reality.*

In classical mechanics, the form of motion is governed by an empirical law of nature. This means that for every physical system, the description of its motion is a result of its subjection under an empirical law. The physical state of a system, however, is completely described by (q_i, p_i). This is because only these quantities are contingent upon the system under consideration *alone*.

One might question: are not the forms of motion contingent upon the system under consideration too? A free particle travels in straight line, whereas a particle in a simple harmonic potential displays periodic motion. Here, it is useful to notice that this contingency is not what the notion physical state attempts to capture primarily. The notion of a physical state attempts to capture the system's 'internal' property, i.e. what can be said to be 'intrinsically' dependent on the system without considerations of other factors, for example the empirical law they are subjected to. The motion, though differs from system to system, is contingent upon the empirical law of motion and thus the concept should not be seen as part of the physical state. More precisely, it is the *evolution* of the physical state in time.

Now if the classical law of motion is not considered as an *empirical law* anymore, then the conceptual significance of motion must change. In that hypothetical scenario, there are two options: i) replace the classical law of motion by another law of motion, and verifies the new law empirically in relevant domains (de Broglie-Bohm theory), ii) give up the possibility of a law of motion being an *empirical law*. In the second scenario, dynamics as a concept altogether will lose its independence and universal applicability. For example, in classical SM, every member in an ensemble must evolve according to the same law of dynamics. This is not necessary if we are to construct a SM type theory for a domain where there is no known empirical law governing the form of motion for all systems.

In the variational approach, the physical picture presupposes the second scenario. This is manifested in the fact that $\mathcal{S}$ alone is not sufficient to determine the dynamics. The dynamics is not determined by the HJ equation solely. By giving up the law of motion as an empirical law, there are two options regarding the role of motion in a physical picture: i)relegate motion to *some* role in the physical explanation (view taken here), ii) abandon the role of motion in the physical explanation of a phenomena.

It seems that the variational approach suggests option (i). The very presence of a HJ ensemble in the variational approach cannot make any sense unless a physical picture is presupposed where motion is assumed to exist for members of the ensemble, albeit in a non-classical form and further, only meaningful at the level of averages. Otherwise, quantities such as $\frac{\partial \mathcal{S}}{\partial q_i}$ are entirely meaningless. The fact that Schrödinger's variational principle retains its form in Schrödinger mechanics suggests that dynamics, and hence motion, play a part in the consideration. However, conceptually both ρ and $\mathcal{S}$ are clearly subsidiary to ψ in this framework. Motivated by the idea to look for a single function for the statistical HJ framework, ψ is given a primary role in the physical picture, in place of motion. But this does not mean that there are *no* role for ρ and $\mathcal{S}$, and hence option (i).

But what kind of physical picture is provided by making ψ primary, in place of motion? Clearly a new empirical law is needed to replace the law of motion as the central law in a physical theory. A very tempting answer arises, if Schrödinger mechanics is interpreted literally as a statistical HJ theory. It follows that ψ *are* the HJ ensembles that are selected by an empirical law of nature. Recall that in statistical HJ theory, ψ is a single function capturing all the possible HJ ensembles that satisfy the following criteria:

1. Possess a probability distribution ρ over it, which satisfies the continuity equation.

2. Members in an ensemble has dynamics governed by $\mathcal{S}$, which satisfies the HJ equation.

Thus solving for ψ in a statistical HJ theory really amounts to capturing all the possibilities in a statistical HJ theory, in the same way $\mathcal{S}$ captures all the dynamical possibilities in HJ theory. Now as we have argued, using ψ in a statistical HJ context is not merely a re-writing of the process of solving the HJ equation and the continuity equation *separately*. Conceptually, solving for ψ takes priority. Further, just as $\mathcal{S}$ captures the empirical law of motion in classical HJ theory, ψ should be regarded as capturing an analogous empirical law in the statistical HJ theory. Now what is subjected to this analogous law? If the motion of individual physical systems is the subject of the empirical law of motion, then the HJ ensembles should be regarded as the subject of this analogous empirical law. This can be summarised as follows:

Law captured by	HJ equation	Schrödinger equation
Single function	$\mathcal{S}$	ψ
What subjects to the law	motion	HJ ensemble
Physical State	(q_i, p_i)	(q_i)

A definitive conclusion from the above comparison seems to be that if we take Schrödigner mechanics as a statistical HJ theory seriously, the central concept of the theory should be the HJ ensembles. Just as classical HJ theory is concerned with the determination of motion at the most general level, Schrödinger mechanics is likewise concerned with the determination of HJ ensembles at the most general level.

Further, while $\mathcal{S}$ itself refers to all the dynamical possibilities, ψ itself also refers to all the possible HJ ensembles which can occur in nature. Recall the crucial point: $\mathcal{S}$ itself do not refer to reality, until specification of the integration constants have been chosen suitably. Likewise, ψ itself also do not refer to reality, until specification of the so-called 'measurement' is given. Thus the analogy here seems to lead to the following: specifying the integration constants in HJ theory, is conceptually *analogous* to selecting a basis in QM which results in the 'collapse'.

To see this more clearly, let us consider the case in HJ theory again. Before we specify the integration constants, we merely have the $\mathcal{S}$ functions which contain all the actual dynamical possibilities. Now, by specifying the meaning of the integration constants, we made a connection with reality, in that a certain possibility contained in $\mathcal{S}$ is being chosen by supplying empirical data, i.e. initial position/momentum/energy...etc. This results in a description of *actual* motion, i.e. $q_i(t)$. In other words, we have 'collapse' all the dynamical possibilities contained in $\mathcal{S}$, to one actual form of motion.

In the same way, the most general solution to Schrödinger equation, namely, the linear superposition of all the solutions, is analogous to $\mathcal{S}$. When we perform a 'measurement', we have specify empirical data into the theory, and thus it is equivalent to having a certain possibility being chosen. Obviously, this results in ψ taking one of the eigenstates. In this sense, the reality of ψ 'enters' only after a specific possibility is chosen.

Finally, the fact that ψ refers to a HJ ensemble and yet can be real after 'measurement' is paradoxical. Recall that HJ ensemble is an ensemble of fictitious particles on fictitious trajectories. In Schrödinger mechanics, this aspect of a HJ ensemble remains the same, even though classical law of motion is not in operation anymore. Thus it seems that if ψ is what is subjected to the empirical law in Schrödinger mechanics, the implication is that HJ ensemble *as a whole*, can be real, even though its parts are fictitious given that there are no possibilities to observe a subatomic particle directly.

I have now sketched an answer for the central question given by the variational approach. The answer essentially rests upon the assumption that the empirical status of motion has changed in subatomic contexts. I will now turn to discuss possible justifications of this assumption.

4.2 Empirical status of 'motion' in Schrödinger mechanics

Recall that in classical mechanics, the law of motion is the central empirical law in the theory. This means that in classical HJ theory, the validity of the framework is justified by the fact that it produces true motion—trajectories—observed in nature. Further, in such a deterministic dynamics, a physical state of a system is provided by (q_i, p_i) and its future evolution completely determined by the specification of the initial state (q_0, p_0). Thus the empirical state of a classical system is given by its configuration and momentum, and the empirical law in classical mechanics is a law of motion. How much do these concepts retain its empirical status?

As mentioned before, in the early 'quantum' experiments only positions can be considered as directly observable. For a subatomic system, we have no direct empirical observation of its motion in space and time. All that we have is a range of initial and final positions. Thus the relevant physical state of the system is not a point in phase space, but in configuration space. Let me justify this further.

In classical mechanics, motion and hence the momentum of a physical system is regarded as directly observable. This means that we can verify the prediction of the theory by observing the configuration and momentum of the physical system directly in experiments. In cases where this is not possible, i.e. trajectories are not observed *directly*, it is obvious that the role of momentum in the physical description of the experiment must differ than that in classical mechanics. Notice that I emphasise on the difference between direct and indirect observation. This is because for example in experiments like the photoelectric effect or Compton scattering, we can still 'observe' the momentum of a quanta *indirectly*. By this I mean something like deducing the quantised momentum via the spectrograph or the photoelectric current. However, by no means this is equivalent to directly observing the trajectory of a particle.[30] Thus for the very least, momentum cannot have the *same* empirical status as in classical physics. This is the reason for distinguishing between the empirical status of configuration q_i and momentum p_i in Schrd̈inger mechanics.

To justify this further, notice that in the early experimental foundations there are a few types of physical phenomena.[31] The first class of phenomena have distributions as its empirical data, i.e. energy distribution, position distribution...etc. In this category we can think of the blackbody radiation. The second class of phenomena have 'interference patterns' as its empirical data. The third class of phenomena have empirical data given by spectrographs. We can think of the absorption/emission spectra of hydrogen and Compton scattering.

Now clearly none of these experiments have the motion of the physical system as its empirical data. For example in the case of the double slit experiment, a pattern on the screen made up of many localisations is obtained from the experiment and require an explanation. However, the double slit experiment involves no empirical observation of the motion of an electron/photon. Thus the distribution of particle on the screen as a concept can have a direct correspondence with empirical observations, whereas the concept 'motion of particles' cannot. Similarly in atomic spectra experiments, the empirical data that requires explanation is the series of lines on a spectrograph. The point is that *in no early quantum phenomena, the motion of the system under description is said to be observed, in the same sense as the motion of, say, planets or pendulums are said to be observed in classical mechanics.*

As a consequence, this justifies the reduction of the 'state' from (q_i, p_i) to q_i only, and thus explain why the sample space in Schrödinger mechanics

[30] We will not go into the discussion about whether there exists new possible definition of the concept of trajectory in quantum mechanics, which enables us to continue to regard momentum as observed directly. We are only showing how the empirical status of momentum must be different to that in classical mechanics.

[31] For more details, see for example [11], chapter 1.

should be the configuration space, not the phase space.[32] The classical law of motion should not treated as an *a priori* empirical law of nature anymore, as in the case of classical SM. This is equivalent to stating that for subatomic physical systems involved in quantum experiments, we cannot preconceive the form of motion they obey. This does not mean the momentum is entirely meaningless. The local momentum $\frac{\partial \mathcal{S}}{\partial q_i}$ can be used as a 'momentum' of a system at the level of averages, and the momentum density d_p are used to determine the correct physical averages in Schrödinger mechanics. Nevertheless, the asymmetry between q_i and p_i in Schrödinger mechanics is thus a well motivated one, at least at an empirical level. And finally, all these considerations will hold *as long as an 'observation of motion of a subatomic particle' is not empirically possible.* However, if it is possible to characterise what an observation of a subatomic particle's motion consists of, then this would decidedly vindicate attempts to re-introduce the an empirical law of 'motion' back into the physical explanation.

5 Conclusion

To conclude, there are certainly substantial motivations behind the variational approach based on the starting point in Schrödinger's first communication. These motivations are established by seeing Schrödinger mechanics as a statistical HJ theory. However, although there seems to be points of analogies between the two theories, the differences are often radical at the conceptual level. The only conclusive result seems to be that ψ must be interpreted as what is subjected to the empirical law of the theory, since it occupies a conceptual position similar, but not identical, to that of $\mathcal{S}$ in classical HJ theory. To see what this entails would require further comparisons between the two functions, especially on the exact analytic discontinuities and similarities. Finally, further investigation is needed to study the validity of the surprising conclusion that ψ refers to a real HJ ensemble, whose parts are fictitious. This is both a philosophical interesting, and potentially theoretically fruitful construct in physics. Afterall, all the empirical evidence we have for the existence of the hydrogen atom points to its 'energy levels' and fine structures. These can be regarded as the property of an ensemble *as a whole*. What could it not be explained by the concept of a real ensemble of fictitious electrons?

[32] This might shed light to why forcing quantum mechanics onto phase space, for example the Wigner-Moyal approach, produces undesirable feature like negative probabilities.

References

[1] David Bohm, "A Suggested Interpretation of the Quantum Theory in terms of "Hidden Variables". I", Phys. Rev., **85**, 166-179 (1952).

[2] David Bohm, "A Suggested Interpretation of the Quantum Theory in terms of "Hidden Variables". II", Phys. Rev., **85**, 180-193(1952).

[3] David Bohm & Basil J. Hiley, *The Undivieed Universe*, Routledge (1993).

[4] Jeremy Butterfield, "On Hamilton-Jacobi Theory as a Classical Root to Quantum Theory", in 'Quo Vadis Quantum Mechanics? *Possible Developments in Quantum Theory in the 21st Century'*, ed. by Elitzur, A.C., Dolev, S., and Kolenda, N., New York: Springer (2004).

[5] Jeremy Butterfield, "David Lewis meets Hamilton and Jacobi", Philosophy of Science, **71**, 10951106 (2004).

[6] David B. Cook, *Schrödinger Mechanics*, World Scientific Lecture Notes in Physics, Vol.28 (1988).

[7] David B. Cook, *Probability and Schrödinger Mechanics*, World Scientific Publishing Co. Pte. Ltd (2002).

[8] Louis de Broglie, ph.D Thesis, *Recherches Sur la Théorie des Quanta*(1923) translated by A.F. Kranklauer (2004).

[9] Louis de Broglie, *Non-Linear Wave Mechanics.* Elsevier Publishing Company (1960).

[10] Louis de Broglie, *The Current Interpretation of Wave Mechanics.* Elsevier Publishing Company (1964).

[11] Giampiero Esposito, Giuseppe Marmo, George Sudarshan, *From Classical to Quantum Mechanics.* Cambridge University Press (2004).

[12] Roman Frigg, "What is Statistical Mechanics?" in *History and Philosophy of Science and Technology*, Eolss, Vol.4, ed. by Carlos Galles, Pablo Lorenzano, Eduardo Ortiz & Hans-Jörg Rheinberger, Isle of Man: Eolss (2010).

[13] Heinrich Hertz, *The Principle of Mechanics.* Dover Publications, Inc., New York (1956).

[14] Peter R. Holland, *The Quantum Theory of Motion: An account of the de Broglie-Bohm causal interpretation of quantum mechanics*. Cambridge University Press (1993).

[15] Christian Joas & Christoph Lehrer, "The Classical Root of Wave Mechanics: Schrödinger's Transformations of the Optical-Mechanical Analogy", Studies in History and Philosophy of Science, Part B, **40**, 4, 338-351 (2009).

[16] Cornelius Lanczos, *The Variational Principles of Mechanics*. University Of Toronto Press (1949).

[17] Rolf Landauer, "Path Concepts in Hamilton-Jacobi Theory", American Journal of Physics, **20**, 6, 363-367 (1952).

[18] Jagdish Mehra & Halmut Rechenberg, *The Historical Development of Quantum Theory, Volume 5, Part I & II*. Springer-Verlag (1987).

[19] Hanno Rund, *The Hamilton-Jacobi Theory in the Calculus of Variations: its role in mathematics and physics*. D. Van Nostrand Company Ltd. (1966).

[20] Erwin Schrödinger, *Collected Papers on Wave Mechanics*, Blackie & Son Ltd (1928).

[21] Richard C. Tolman, *The Principle of Statistical Mechanics*. Dover Publications Inc., New York (1979).

[22] Antony Valentini & Guido Bacciagaluppi, *Quantum Theory at the Crossroad: Reconsidering the 1927 Solvay Conference*. Cambridge University Press (2009).

[23] Timothy C. Wallstrom, "Inequivalence between the Schrödinger equation and the Madelung Hydrodynamic equations", Phys. Rev. A, **49**, 3, 143-182 (1994).

[24] Linda Wessels, "Schrödinger's route to Wave Mechanics", Studies in History and Philosophy of Science, Part A, **10**, 4, 311-340 (1979).

[25] Wolfgang Yourgrau & Stanley Mandelstam, *Variational Principles in Dynamics and Quantum Theory, Third Edition*. Sir Isaac Pitman & Sons Ltd. (1968).